

Energy Technology

Supporting Information

Implications of Exceptional Material Kinetics on Thermochemical Fuel Production Rates

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Table S1. Digitized enthalpy and entropy values for ceria used for calculations.^[1]

δ (unitless)	ΔH (kJ mol O ⁻¹)	ΔS (J mol O ⁻¹ K ⁻¹)
0.00107	488.0935	312.9523
0.0017	482.8914	298.5588
0.00269	482.0101	288.9031
0.00428	480.6786	279.1119
0.00656	474.5615	266.3638
0.01059	468.0005	252.3598
0.01715	459.0274	236.9652
0.02169	453.19	230.0771
0.02673	447.8834	222.9187
0.0338	441.0812	214.319
0.04288	433.5553	204.946
0.05448	424.341	195.2278
0.0681	415.6091	186.0601
0.08474	405.6229	174.8597
0.107	396.6498	163.3978
0.136	389.8476	152.1058
0.155	390.5713	148.1031
0.171	394.6719	146.0936
0.2	403.8862	142.9631
0.215	407.5044	141.3439
0.243	412.0874	138.8628
0.27	414.982	138.1578

Table S2. Digitized enthalpy and entropy values for Zr10 used for calculations.^[2]

δ (unitless)	ΔH (kJ mol O ⁻¹)	ΔS (J mol O ⁻¹ K ⁻¹)
0.01	342.57888	192.50591
0.02	355.23261	185.12768
0.03	359.50464	178.011355
0.04	363.062385	172.793935
0.05	366.082845	169.258105
0.06	368.70598	166.532235
0.07	377.79676	169.24751
0.08	378.847425	166.979355
0.09	378.971145	164.314505
0.1	379.25659	161.88976
0.11	380.839785	160.457015
0.12	378.81605	156.65135
0.13	377.251105	153.247865
0.14	375.407055	149.55118
0.15	373.563005	145.85449
0.16	371.00868	141.50397
0.17	374.714275	141.214675
0.18	371.70374	136.496625
0.19	368.39866	131.52944
0.2	364.88618	126.40833
0.21	365.97181	124.241195
0.22	363.043605	119.55942
0.23	362.920675	116.679845
0.24	360.861385	112.725325
0.25	360.502065	109.952175
0.26	362.104175	108.54904

Table S3. Digitized enthalpy and entropy values for Zr20 used for calculations.^[2]

δ (unitless)	ΔH (kJ mol O ⁻¹)	ΔS (J mol O ⁻¹ K ⁻¹)
0.01	282.8653	167.89205
0.02	312.344045	171.62324
0.03	325.204045	168.96755
0.04	331.913705	165.07843
0.05	334.68151	160.246375
0.06	343.834905	161.30268
0.07	349.719545	160.515305
0.08	354.2287	159.15464
0.09	358.475365	158.321575
0.1	361.82858	157.099895
0.11	368.65035	158.681995
0.12	370.23876	156.85182
0.13	371.57031	154.92527
0.14	374.950265	154.47687
0.15	376.699115	152.955675
0.16	377.4394	150.753845
0.17	376.80357	147.60528
0.18	376.47762	144.25562
0.19	376.51996	140.907695
0.2	375.541605	136.769685
0.21	372.574045	131.30143
0.22	369.428475	125.589135
0.23	360.91945	116.50832
0.24	379.9061	124.324575
0.25	389.34742	125.80795
0.26	396.365145	125.56901

References

- [1] R. J. Panlener, R. N. Blumenthal, J. E. Garnier, *J. Phys. Chem. Solids* **1975**, 36, 1213–1222.
- [2] Y. Hao, C.-K. Yang, S. M. Haile, *Chem. Mater.* **2014**, 26, 6073–6082.